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# CALCULATIONS ON AUTOIONIZATION OF THE $^4P_{5/2}{}^\circ$ STATE OF He$^-$†

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The lifetime against autoionization of the $^4P_{5/2}{}^\circ$ state of He$^-$ is calculated using an accurate description of the initial- and final-state wave functions. In these calculations the initial $^4P_{5/2}{}^\circ$ state is represented by a variational wave function consisting of several angular configurations. The final $^2F_{5/2}{}^\circ$ continuum state is obtained by polarized-orbital theory. A lifetime of $4.55\times10^{-4}$ sec is predicted which is in good agreement with the most recent experimental measurement.

In this Letter, we present the results of a calculation of the autoionization lifetime of the $^4P_{5/2}{}^\circ$ state of He$^-$ using more accurate descriptions of both the initial and final states than have been used together in previous calculations.[1-3]

The $^4P_{5/2}{}^\circ$ state of a three-electron system is stable against all but the spin-spin interaction, through which it will autoionize into the $(1s)^2kf\,^2F_{5/2}{}^\circ$ continuum. The lifetime towards autoionization is given to first order in the spin-spin interaction by[4]

$$\tau=(\tau_0/\pi)|\langle\Psi_k|H'|\Phi\rangle|^{-2}, \tag{1}$$

where $\Phi$ is the initial $^4P_{5/2}{}^\circ$ state and $\Psi_k$ is the adjacent $^2F_{5/2}{}^\circ$ continuum. $H'$ is the spin-spin interaction which for the purposes of this calculation may be written

$$H'=\tfrac{1}{2}\alpha^2\textstyle\sum_{i>j}(\vec{\sigma}_i\cdot\nabla_i)(\vec{\sigma}_j\cdot\nabla_j)r_{ij}^{-1}. \tag{2}$$

Atomic units of energy in rydbergs are used. $\alpha$ is the fine-structure constant and $\tau_0$ is the unit of atomic time.

The initial- and final-state wave functions $\Phi$ and $\Psi_k$ are ideally exact eigenstates of the zero-order Hamiltonian for the three-electron system,

$$H_0=-\nabla_1{}^2-\nabla_2{}^2-\nabla_3{}^2-4/r_1-4/r_2-4/r_3+2/r_{12}+2/r_{13}+2/r_{23}. \tag{3}$$

In actuality, though, only approximate solutions are known, and so accurate estimation of the autoionization lifetime is contingent upon the approximations used for $\Phi$ and $\Psi_k$. The thesis of the present calculation is to use functions which are accurate approximations to the eigenfunctions of $H_0$. The resulting lifetime estimate will then be essentially correct to $O(\alpha^2)$.[2]

The most accurate approximation to the eigenstate of $H_0$ for the initial $^4P_{5/2}{}^\circ$ state presently available has been found by Weiss.[5] This function was obtained using the variational principle and consists of a superposition of Hartree-Fock–type configurations with 28 different choices of the principal and orbital quantum numbers $n_1l_1$, $n_2l_2$, $n_3l_3$ for the bound electrons. The binding energy for this function is

0.067 eV with respect to the $2^3S$ state of He. The most recent measurement of the affinity of $\mathrm{He}^-$ was obtained by Brehm, Gusinow, and Hall using laser photodetachment techniques.[6] They found the affinity to be 0.080 ± 0.002 eV. We have used Weiss's multiconfiguration wave function to represent the initial ${}^4P_{5/2}{}^\circ$ state in the calculations reported in this Letter.

The final-state wave function $\Psi_k$ is analogous to that for the elastic scattering of an electron with energy

$$k^2 = E({}^4P_{5/2}{}^\circ) - E({}^1S_0) \tag{4}$$

from helium in its $(1s)^2\,{}^1S_0$ ground state. An accurate description of this scattering process has been given recently by Callaway et al.[7] under what they call the extended-polarization-potential (EP) method.

The EP method treats the electron-atom interaction on the basis of Hartree-Fock theory, giving special emphasis to a proper description of the long-range-distortion interactions. For $f$-wave scattering by helium in a total ${}^2F_{5/2}{}^\circ$ configuration, the final-state wave function in the EP approximation may be written

$$\Psi_k(1,2,3) = 3^{-1/2}\sum \psi^{(d)}(1,2;3)S(1,2)\psi_{kf}(3), \tag{5}$$

where

$$\psi^{(d)}(1,2;3) = \psi_0(\vec{r}_1)\psi_0(\vec{r}_2) + \psi_0(\vec{r}_1)\chi(\vec{r}_2;\vec{r}_3) + \psi_0(\vec{r}_2)\chi(\vec{r}_1;\vec{r}_3). \tag{6}$$

The summation in Eq. (5) is over all cyclic permutations of the indices 1, 2, and 3. $S(1,2)$ is the singlet spin function for bound electrons 1 and 2, and $\psi_{kf}$ is the wave function for the continuum electron,

$$\psi_{kf}(3) = [u_{kf}(r_3)/r_3][(6/7)^{1/2}Y_3{}^3(\hat{r}_3)\beta_3 - (1/7)^{1/2}Y_3{}^2(\hat{r}_3)\alpha_3]. \tag{7}$$

$\psi_0$ is the Hartree-Fock 1$s$ wave function for helium, and $\chi$ is a correction to this to account for the distortion induced in the atom by the continuum electron.

The correction $\chi$ is determined by perturbed Hartree-Fock theory under the adiabatic approximation. The resulting $\chi$ is decomposed into multipole components,

$$\chi(\vec{r}_i;\vec{r}_j) = \sum_l \chi_l(\vec{r}_i;\vec{r}_j) = \sum_l F_l(r_i;r_j)P_l(\hat{r}_i\cdot\hat{r}_j)\psi_0(\vec{r}_i). \tag{8}$$

The first three of these ($l = 0, 1, 2$), which are all that are used in the present work, are described elsewhere.[7,8]

The reduced radial part $u_{kf}$ of the continuum electron wave function is a solution of the equation

$$\left(-\frac{d^2}{dr_3{}^2} + \frac{12}{r_3{}^2} - \frac{4}{r_3} + 4\langle\psi_0(2)|r_{23}{}^{-1}|\psi_0(2)\rangle + V_p(r_3) - k^2\right)u_{kf}(r_3) = \frac{2}{7}\int u_{1s}(r_2)\frac{r_<{}^3}{r_>{}^4}u_{kf}(r_2)dr_2u_{1s}(r_3), \tag{9}$$

where $u_{1s}(r) = [4\pi]^{1/2}r\psi_0(\vec{r})$ and $V_p$ is a potential representing the induced-distortion interaction. In the EP method, $V_p$ is a sum of the adiabatic polarization potential plus a repulsive correction to account for the finite velocity of the external electron.[7] The solution of Eq. (9) is normalized asymptotically to

$$u_{kf}(r) \xrightarrow[r\to\infty]{} (\pi k)^{-1/2}\sin(kr - \tfrac{3}{2}\pi + \eta_3), \tag{10}$$

where $\eta_3$ is the phase shift.

Upon substituting the final-state wave function from Eq. (5) into the matrix element in Eq. (1) the result separates naturally into two parts, the first of which involves only the undistorted portion of the final-state wave function $\psi_0$, and the second containing the correction $\chi$. When $\chi$ is decomposed into multipole components the second part separates further into a term involving only the monopole ($l = 0$) component of $\chi$, another involving only the dipole ($l = 1$) component, and so on. We have calculated the undistorted, monopole, and dipole terms only and listed the resulting matrix-element components in Table I. We also list in the last column of the table the lifetimes resulting from the matrix elements listed.

We have separated the data in Table I according to the approximations used in determining the continuum wave function from Eq. (9). The first entry (static-exchange) corresponds to complete neglect of the induced distortion effects, which results if $\chi$ and $V_p$ are set to zero throughout. This calculation was done for reference purposes only and repeats Laughlin and Stewart's latest calculation.[9] The next entries were calcu-

Table I. Transition matrix-element components and lifetime for the ${}^4P_{5/2}{}^\circ$ state of $He^-$.

| Final-state wave function | Matrix-element components ($10^{-8}$ a.u.) Undistorted | Monopole | Dipole | Lifetime $\tau$ ($10^{-4}$ sec) |
|---|---|---|---|---|
| Static-exchange | 11.90 | | | 5.44 |
| Adiabatic-exchange-dipole | 12.08 | | | 5.27 |
| | | | +0.60 | 4.78 |
| Extended-polarization-potential | 12.04 | | | 5.31 |
| | | +0.37 | +0.60 | 4.55 |
| Experiment: Nicholas *et al.* (Ref. 10) | 12.04 | | | 0.18 ± 0.027 |
| Blau *et al.* (Ref. 13) | 12.04 | | | 3.45 ± 0.90 |

lated under the adiabatic-exchange-dipole approximation which results if only the dipole component of $\chi$ is retained in the matrix element and only the dipole component of the adiabatic polarization potential is used for $V_p$ in Eq. (9). The extended-polarization-potential results were obtained as outlined above.

The results of our calculations as listed in Table I show that the major effects of the distortion interaction on the predicted lifetime result from including the perturbation correction $\chi$ in the matrix element. A reduction of at most only 3% in $\tau$ is obtained by using the distorted continuum wave function in the undistorted matrix element. A total reduction of 16% in $\tau$ is obtained by including the monopole and dipole distortion matrix-element components as well. However, the trend of the monopole and dipole matrix-element components indicates that higher multipole components may also be significant. These have yet to be examined.

There are at present two conflicting experimental results for the lifetime of $He^-$ as listed in Table I. The first was obtained by Nicholas, Trowbridge, and Allen by observing the decay of $He^-$ ions through 1- and 2-m drift tubes.[10] The second experimental result was obtained by Blau, Novick, and Weinflash by observing the decay of $He^-$ within a 10-m drift tube.[11] When $He^-$ ions in a ${}^4P_J$ state are formed by double charge exchange between $He^+$ ions and a neutral species, a distribution of the possible total angular momentum states $J=\frac{1}{2}$, $\frac{3}{2}$, and $\frac{5}{2}$ will result. The states with $J=\frac{1}{2}$ and $\frac{3}{2}$ can decay by both spin-orbit and spin-spin interactions and thus are expected to have lifetimes at least an order of magnitude smaller than the $J=\frac{5}{2}$ state.[12] It appears that the measurements by Nicholas, Trowbridge, and Allen represent only a mean lifetime for all three ${}^4P_J{}^\circ$ states of $He^-$ because of their relatively short drift-path lengths.[13]

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